Polygamma theory, the Li/Keiper constants, and validity of the Riemann Hypothesis

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Abstract

The Riemann hypothesis is equivalent to the Li criterion governing a sequence of real constants $\{\lambda_k\}_{k=1}^\infty$, that are certain logarithmic derivatives of the Riemann xi function evaluated at unity. We investigate a related set of constants c_n, $n = 1, 2, \ldots$, showing in detail that the leading behaviour $(1/2) \ln n$ of λ_n/n is absent in c_n. Additional results are presented, including a novel explicit representation of c_n in terms of the Stieltjes constants γ_j. We conjecture as to the large-n behaviour of c_n. Should this conjecture hold, validity of the Riemann hypothesis would follow.

Key words and phrases

Li/Keiper constants, Riemann zeta function, Riemann xi function, logarithmic derivatives, Riemann hypothesis, Li criterion, Laurent expansion, Stieltjes constants

Introduction

The Riemann hypothesis is equivalent to the Li criterion governing the sequence of real constants $\{\lambda_k\}_{k=1}^{\infty}$, that are certain logarithmic derivatives of the Riemann xi function evaluated at unity. This equivalence results from a necessary and sufficient condition that the logarithmic derivative of the function $\xi[1/(1-z)]$ be analytic in the unit disk, where ξ is the Riemann xi function. The Li equivalence [22] states that a necessary and sufficient condition for the nontrivial zeros of the Riemann zeta function to lie on the critical line Re $s = 1/2$ is that $\{\lambda_k\}_{k=1}^{\infty}$ is nonnegative for every integer k.

This paper is a further contribution to our research program to characterize the Li (Keiper [19]) constants [22, 23]. We have previously rederived [5, 6] an arithmetic formula [3] for these constants, and described how it could be used to estimate them. Elsewhere, among several other results, we have examined summatory properties of the Li and Stieltjes constants, and investigated the η_j coefficients appearing in the logarithmic derivative of the zeta function about $s = 1$ [7]. In particular, a key feature of the sequence $\{\eta_j\}_{j=0}^{\infty}$ is now known: it possesses strict sign alternation [7].

In this paper, we investigate a related set of constants [28] c_n, $n = 1, 2, \ldots$, that might be thought of as reduced Li/Keiper constants. We show in detail that the leading behaviour $(1/2)\ln n$ of λ_n/n is absent in c_n. What remains in c_n is a direct manifestation of fundamental properties of the zeta function. Thus, c_n can be variously interpreted as reflecting the nontrivial zeros, or the η_j constants. We present

additional analytic results, including an explicit representation of c_n in terms of the Stieltjes constants γ_k. We conjecture on the precise order of c_n in n, we comment on the nature of the logarithmic derivative of the zeta function, and we briefly discuss possible interpretations of some of our results.

The Gamma function is important in the theory of the Riemann zeta function– for instance it is needed to complete ζ to the ξ function. The Gamma function figures prominently in the functional equation for the zeta function, thereby largely determining the location of the trivial zeros and other analytic properties. Hence the digamma function appears in the logarithmic derivative of the xi function, and higher derivatives introduce the polygamma functions $\psi^{(j)}$ [2]. Portions of the theory of this family of functions are very important in much of this paper. We have also made extensive use of the properties of $\psi^{(j)}$ in previous works [5, 6, 7].

Our approach is explicit and very much in the spirit of constructivistic mathematics. Indeed, our work may be much more explicit than what would have been thought possible just a few years ago.

From improved numerical calculation to height $T \simeq 2.38 \times 10^{12}$ [13], it is now known that at least the first ten trillion complex zeros of the zeta function lie on the critical line. For our purposes, this effectively ensures that approximately the first 10^{26} λ_k's are nonnegative, and this fact may have significant implications for our investigations. For instance, it may very well turn out that working asymptotically in k will suffice in our research program.

The Li equivalence is by itself a qualitative reformulation of the Riemann hypothesis. The Riemann hypothesis does not of itself dictate the exact nature of the Li/Keiper constants. In fact, one can easily formulate conjectures on the nature and order of the Li/Keiper constants that are then stronger than the Riemann hypothesis. These observations indicate that the Riemann hypothesis may be verifiable without knowing the optimal order or other properties of the Li/Keiper constants that would more fully characterize them.

It is possible to use our approach also in pursuit of confirmation of the extended and generalized Riemann hypotheses. The corresponding λ constants have been defined for Dirichlet and Hecke L-functions and other zeta functions [23], and the same leading behaviour $O(j \ln j)$ has been found [6]. Our attention here is strictly with the classical zeta function.

Preliminary Relations

We first recall some notation, introduce some definitions, and present an important Lemma for subsequent developments. We introduce the function [28]

$$F(z) = \ln\left[\frac{z}{1-z}\zeta\left(\frac{1}{1-z}\right)\right], \tag{1}$$

whose analyticity in the unit disc $|z| < 1$ in the complex plane is equivalent to the Riemann hypothesis. Then, should the power series

$$F(z) = \sum_{n=0}^{\infty} c_n z^n \tag{2}$$

converge for $|z| < 1$, the Riemann hypothesis follows. In short order, one verifies that

the c_n are real constants, $c_0 = 0$, and $c_1 = \gamma$, the Euler constant. Therefore, we may write

$$F(z) = \gamma z + \sum_{n=2}^{\infty} c_n z^n. \tag{3}$$

This paper investigates the behaviour of the constants c_n. The importance of this subject is clear: from any subexponential bound on them the Riemann hypothesis follows [3, 28]. Indeed, in this paper we additionally conjecture the true order of the constants $|c_n|$, such that this conjecture is stronger than the Riemann hypothesis itself.

Suppose we knew that $F(z)$ is analytic and univalent within the unit disc. Then the function $F(z)/\gamma$, satisfying $F(0)/\gamma = 0$ and $F'(0)/\gamma = 1$, is schlicht, fulfills the conditions for the Bieberbach conjecture [10] to hold, and thus we would have $|c_n| \leq \gamma n$ for all $n = 1, 2, \ldots$. This shows the self consistency of the complex analysis involved. In fact, any direct application to the Bieberbach conjecture is thwarted due to the essential singularity in F, making it highly non-univalent.

Related to a prefactor in Eq. (1), $k(z) = z/(1-z)^2$ is the Koebe function, and $k_\alpha(z) = z/(1-\alpha z)^2$ with $|\alpha| = 1$ are rotations of it. These are the only functions for which equality holds in the conclusion of the Bierberbach conjecture. The history of the Bieberbach conjecture shows that it is easier to obtain results about the logarithmic coefficients of a univalent function rather than for the coefficients of the function itself [20], and the approach of Smith [28] seems to fit within this framework.

The classical Laurent expansion of the Riemann zeta function about the unique

pole at $s = 1$ introduces the Stieltjes constants γ_k [17, 16, 25, 26], with $\gamma_0 = \gamma$. We have

$$\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n (s-1)^n, \tag{4}$$

where the Stieltjes constants can be written in the form

$$\gamma_k = \lim_{N \to \infty} \left(\sum_{m=1}^{N} \frac{1}{m} \ln^k m - \frac{\ln^{k+1} N}{k+1} \right). \tag{5}$$

and several other forms have been given [16]. It is clear that the c_n's are multinomials in the Stieltjes constants, and that c_n contains terms $-(-1)^n \gamma^n / n$ and $-(-1)^n \gamma_{n-1}/(n-1)!$. Indeed, we are able to write much more, giving, for instance, an explicit formula for c_n in terms of the γ_k's. Once again, we may therefore observe that sufficient estimation of the Stieltjes constants would provide verification of the Riemann hypothesis.

We discuss these connections with the Stieltjes constants in a later section. For the moment, we simply point out that Appendix A contains explicit formulae for the first few c_n's in terms of them.

The conformal map introducing the Li/Keiper constants and the coefficients c_n is a natural one. This map $z = 1 - 1/s \leftrightarrow s = 1/(1-z)$ takes the right-half plane Re $s > 1/2$ to the interior of the unit circle in the complex z-plane. Just this sort of mapping arises in the theory of finite fields, whose zeta functions have zeros on a circle in the complex plane [31, 15, 4, 30]. We recall that Weil proved the Riemann hypothesis holds for nonsingular curves over a finite field [31], while Deligne

established the validity of Weil's conjectures for generalized hypersurfaces that may include intersections of hypersurfaces [15].

We first present the explicit connection between the Li/Keiper constants and the constants c_n. We have

Lemma 1

$$\frac{\lambda_n}{n} = c_n + \frac{1}{n} - \frac{1}{2}\ln\pi + d_n, \qquad n \geq 1, \tag{6}$$

where d_n is the coefficient of z^n of the function $\ln\Gamma[1/2(1-z)]$, and Γ is the Gamma function. That is,

$$d_n = \frac{1}{n!}\frac{d^n}{dz^n}\ln\Gamma\left[\frac{1}{2(1-z)}\right]_{z=0}. \tag{7}$$

We will present not only d_n, but the derivatives themselves in this equation. We then estimate d_n in n and demonstrate that the leading behaviour of λ_n/n in Eq. (6) exactly cancels it. This is highly supportive of a decrease of $|c_n|$ with n, and of the conclusion that the Riemann hypothesis should hold. Since we have previously conjectured as to the subdominant behaviour of the Li constants [6, 7], we thereby have an immediate conjecture for $|c_n|$.

Before proving the Lemma and going on to expressions for d_n, we give some brief background on the Li (or Keiper) constants. The function ξ is determined from ζ by the relation [9, 11, 17, 18, 29, 27]

$$\xi(s) = \frac{s}{2}(s-1)\pi^{-s/2}\Gamma\left(\frac{s}{2}\right)\zeta(s), \tag{8}$$

and satisfies the functional equation $\xi(s) = \xi(1-s)$. The sequence $\{\lambda_n\}_{n=1}^{\infty}$ is defined

by

$$\lambda_n = \frac{1}{(n-1)!} \frac{d^n}{ds^n} [s^{n-1} \ln \xi(s)]_{s=1}. \tag{9}$$

The λ_j's are connected to sums over the nontrivial zeros of $\zeta(s)$ by way of [19, 22]

$$\lambda_n = \sum_\rho \left[1 - \left(1 - \frac{1}{\rho}\right)^n\right], \tag{10}$$

and

$$\lambda_1 = -\frac{\ln \pi}{2} + \frac{\gamma}{2} + 1 - \ln 2. \tag{11}$$

In the representation [3, 5, 6, 7]

$$\frac{\lambda_n}{n} = \frac{1}{n} S_1(n) + \frac{1}{n} S_2(n) - \frac{1}{2}(\gamma + \ln \pi + 2\ln 2), \tag{12}$$

the sum

$$S_1(n) \equiv \sum_{m=2}^n (-1)^m \binom{n}{m} (1 - 2^{-m})\zeta(m), \qquad n \geq 2, \tag{13}$$

has been characterized [6]:

$$\frac{n}{2}\ln n + (\gamma - 1)\frac{n}{2} + \frac{1}{2} \leq S_1(n) \leq \frac{n}{2}\ln n + (\gamma + 1)\frac{n}{2} - \frac{1}{2}. \tag{14}$$

Further bounds on $S_1(n)$ have been developed by applying Euler-Maclaurin summation to all orders [6].

For the sum

$$S_2(n) \equiv -\sum_{m=1}^n \binom{n}{m} \eta_{m-1}, \tag{15}$$

the constants η_j can be written as

$$\eta_k = \frac{(-1)^k}{k!} \lim_{N\to\infty} \left(\sum_{m=1}^N \frac{1}{m} \Lambda(m) \ln^k m - \frac{\ln^{k+1} N}{k+1}\right), \tag{16}$$

and Λ is the von Mangoldt function [11, 17, 18, 29, 27], such that $\Lambda(k) = \ln p$ when k is a power of a prime p and $\Lambda(k) = 0$ otherwise. The constants η_j enter the expansion around $s = 1$ of the logarithmic derivative of the zeta function,

$$\frac{\zeta'(s)}{\zeta(s)} = -\frac{1}{s-1} - \sum_{p=0}^{\infty} \eta_p (s-1)^p, \qquad |s-1| < 3, \tag{17}$$

and the corresponding Dirichlet series valid for Re $s > 1$ is

$$\frac{\zeta'(s)}{\zeta(s)} = -\sum_{n=1}^{\infty} \frac{\Lambda(n)}{n^s}. \tag{18}$$

The constants η_j, with $\eta_0 = -\gamma$, have been written explicitly in terms of the Stieltjes constants [7, 24], a point on which we return later. Additionally, we recently proved the strict sign alternation of the sequence $\{\eta_j\}_{j=0}^{\infty}$ [7].

Now that the sum $S_2(n)$ has been introduced, we may present the exact relation

Lemma 2

$$\frac{S_2(n)}{n} = c_n. \tag{19}$$

For, from Eq. (2) it follows that $c_n = (1/n!)(d^n/dz^n)F(z)|_{z=0}$, and from Eqs. (8) and (9) we have

$$\begin{aligned} S_2(n) &= \frac{1}{(n-1)!}\frac{d^n}{ds^n}\left[s^{n-1}\ln[(s-1)\zeta(s)]\right]_{s=1} \\ &= \sum_{m=1}^{n}\binom{n}{m}\frac{1}{(m-1)!}\frac{d^m}{ds^m}\ln\left[(s-1)\zeta(s)\right]_{s=1}. \end{aligned} \tag{20}$$

Under the mapping $s(z) = 1/(1-z)$, derivatives transform as $d/dz = s^2 d/ds$, and the Lemma follows.

Proof of Lemma 1 and expressions for d_n

From Eqs. (1) and (8) we have

$$\ln\xi\left(\frac{1}{1-z}\right) = F(z) - \ln(1-z) + \frac{1}{2(z-1)}\ln\pi + \ln\Gamma\left[\frac{1}{2(1-z)}\right]. \tag{21}$$

Since we have [22, 23]

$$\ln\xi\left(\frac{1}{1-z}\right) = \sum_{n=1}^{\infty}\frac{\lambda_n}{n}z^n, \tag{22}$$

the expansion of Eq. (21) in powers of z readily yields Eq. (6). (For the latter equation, we have used the convention $\xi_{Li}(z) = 2\xi(z)$, such that $\xi_{Li}(0) = 1$, in place of $\xi(z)$. Otherwise, Eq. (6) will have another minor term $-\ln 2$.)

From Lemmas 1 and 2 it follows that

Corollary

$$\frac{S_1}{n} - \frac{\gamma}{2} = \frac{1}{n} + d_n. \tag{23}$$

We next have

Lemma 3

$$\frac{d^n}{dz^n}\ln\Gamma\left[\frac{1}{2(1-z)}\right] = \frac{1}{2}\frac{d^{n-1}}{dz^{n-1}}\frac{1}{(1-z)^2}\psi\left[\frac{1}{2(1-z)}\right]$$
$$= \frac{1}{2}\sum_{j=0}^{n-1}\binom{n-1}{j}\frac{(n-j)!}{(1-z)^{n-j+1}}\frac{d^j}{dz^j}\psi\left[\frac{1}{2(1-z)}\right]$$
$$= \frac{1}{2}\left\{\frac{n!}{(1-z)^{n+1}}\psi\left[\frac{1}{2(1-z)}\right] + \sum_{j=1}^{n-1}\binom{n-1}{j}\frac{(n-j)!}{(1-z)^{n+1}}\sum_{\ell=1}^{j}\binom{j}{\ell}\frac{(j-1)!}{(\ell-1)!}\frac{1}{2^\ell(1-z)^\ell}\psi^{(\ell)}\left[\frac{1}{2(1-z)}\right]\right\}, \tag{24}$$

where ψ is the digamma function and $\psi^{(j)}$ is the polygamma function.

We mention two proofs of this Lemma. The key ingredient is knowing how to write the successive derivatives of the digamma factor. This can be accomplished by applying the Faa di Bruno formula for the nth derivative of a composite function. We have

$$\frac{d^n}{dz^n}\psi\left[\frac{1}{2(1-z)}\right] = \frac{1}{(1-z)^n}\sum_{j=1}^{n}\binom{n}{j}\frac{(n-1)!}{(j-1)!}\frac{1}{2^j(1-z)^j}\psi^{(j)}\left[\frac{1}{2(1-z)}\right]. \tag{25}$$

This equation is just a slight extension of a formula for the derivatives of a function $\theta(1/x)$ [8]. Equation (25), when used with the product rule, completes the Lemma.

Another method can be based upon the expansion [1, 2]

$$\Gamma(z) = \frac{1}{z}\exp\left[-\gamma z + \sum_{k=2}^{\infty}\frac{(-1)^k\zeta(k)}{k}z^k\right], \tag{26}$$

giving

$$\ln\Gamma\left[\frac{1}{2(1-z)}\right] = \ln 2 - \sum_{n=1}^{\infty}\frac{z^n}{n} - \frac{\gamma}{2}\sum_{n=0}^{\infty}z^n + \sum_{k=2}^{\infty}\frac{(-1)^k\zeta(k)}{k2^k}\left(\sum_{j=0}^{\infty}z^j\right)^k. \tag{27}$$

Expanding the powers of power series on the right side returns us to the Lemma. Afterall, we have the relation

$$\psi^{(j)}\left(\frac{1}{2}\right) = (-1)^{j+1}j!(2^{j+1}-1)\zeta(j+1), \qquad j \geq 1, \tag{28}$$

and this is very helpful in rewriting the constants d_n below.

From Eqs. (25) and (28) we have an exact reformulation of digamma derivatives of interest:

Lemma 4

$$\frac{d^n}{dz^n}\psi\left[\frac{1}{2(1-z)}\right]_{z=0} = n!\sum_{m=1}^{\infty}\frac{1}{m^2}\left[2\left(1-\frac{1}{m}\right)^{n-1} - \frac{1}{2}\left(1-\frac{1}{2m}\right)^{n-1}\right]. \tag{29}$$

This Lemma follows by setting $z = 0$ in Eq. (25), inserting Eq. (28), using the Dirichlet series for the zeta function, and reordering the double sum. The use of a derivative relation of a binomial sum completes the work.

We are in position to write compact, yet exact, expressions for the constants d_n:

Lemma 5

$$d_n = \frac{1}{2}\psi\left(\frac{1}{2}\right) + \frac{1}{2n}\sum_{j=1}^{n-1}(n-j)\sum_{m=1}^{\infty}\frac{1}{m^2}\left[2\left(1-\frac{1}{m}\right)^{j-1} - \frac{1}{2}\left(1-\frac{1}{2m}\right)^{j-1}\right]$$

$$= \frac{1}{2}\psi\left(\frac{1}{2}\right) + \frac{1}{2n}\sum_{m=1}^{\infty}\left[2\left(1-\frac{1}{m}\right)^{n} - 2\left(1-\frac{1}{2m}\right)^{n} + \frac{n}{m}\right], \qquad n \geq 1, \tag{30}$$

where $\psi(1/2)/2 = -\gamma/2 - \ln 2$. The first line of the Lemma follows from the combination of the results of Lemmas 2 and 3, and the second line follows from application of finite geometric series.

High order approximation for the constants d_n

There are many ways in which to obtain highly accurate approximations to d_n for large values of n. The upshot is

Lemma 6

$$\ln\Gamma\left[\frac{1}{2(1-z)}\right] \simeq \frac{1}{2}\ln\pi + \frac{1}{2}\sum_{j=1}^{\infty}\left[\psi(j) + \gamma - \ln 2 - 1\right] z^j. \tag{31}$$

That is, for $j >> 1$ we have

$$d_j = \frac{1}{2}\left[\ln j - \frac{1}{2j} - \frac{1}{12j^2} + \gamma - \ln 2 - 1 + O\left(\frac{1}{j^4}\right)\right]. \tag{32}$$

In connection with Eq. (31), we recall the value of the digamma function at integer argument in terms of harmonic numbers H_n: $\psi(n) = H_{n-1} - \gamma$.

We indicate a couple of approaches for obtaining Lemma 6. One is based upon using the integral corresponding to the summation on the second line of Eq. (30). It turns out that this integral, $I_1(n)$, was extensively studied in Appendix A of Ref. [6], and we have taken over the results.

In another method, we apply Euler-Maclaurin summation to the sum over m on the first line of Eq. (30). In doing so, we put

$$f(m) \equiv \frac{1}{m^2}\left[2\left(1-\frac{1}{m}\right)^{n-1} - \frac{1}{2}\left(1-\frac{1}{2m}\right)^{n-1}\right], \tag{33}$$

such that $f(1) = -2^{-n}$, $f(\infty) = 0$, and we have the elementary integral

$$\int_1^\infty f(k)dk = \frac{1+2^{-n}}{n}. \tag{34}$$

Therefore we obtain

$$\frac{d^n}{dz^n}\psi\left[\frac{1}{2(1-z)}\right]_{z=0} \simeq n!\left(\frac{1+2^{-n}}{n} - 2^{-n-1}\right). \tag{35}$$

Then the sum over j can be performed in Eq. (30). In either approach, we discard any terms in the final result that are exponentially small in n, such as $2^{1-n}/n$.

Of note, all terms in d_n beyond the leading logarithmic dependence are in terms of integral powers of $1/n$–there is no algebraic dependence upon n.

Relations and formulae for c_n

With the aid of Cauchy's integral formula, the c_n's can be written as

$$c_n = \frac{1}{2\pi i}\int_C \frac{F(z)}{z^{n+1}}dz, \tag{36}$$

where C is a simple closed contour about the origin, and this can serve as the basis of a numerical method [28]. If C is a circle of radius r about the origin, then $c_n = r^{-n} \int_0^1 F(re^{2\pi i\phi})e^{-2\pi in\phi}d\phi$, and this invites the use of fast Fourier transform for evaluation.

The combination of the result of Lemma 5 with Eqs. (6), (12), and (14) shows that $c_n = S_2(n)/n + O(1/n)$, and Lemma 2 gives the strengthening to $c_n = S_2(n)/n$. Since we have previously conjectured that $|S_2(n)| = O(n^{1/2+\varepsilon})$ for $\varepsilon > 0$, we have

Conjecture

$$|c_n| = O\left(\frac{1}{n^{1/2-\varepsilon}}\right), \tag{37}$$

where $\varepsilon > 0$ but is otherwise arbitrary. That is, we anticipate that the magnitudes $|c_n|$ decrease nearly as the square root of n for large n. In Figure 1 we compare such a decrease with available numerical evidence [28, 24, 6]. Figure 1 contains a semilogarithmic plot of $|c_n|$ versus n, together with a curve corresponding to $6/\pi^2\sqrt{n}$. For this limited set, after a few initial values, the latter curve appears to provide a consistent upper bound. In light of the von Koch result on the Riemann hypothesis that $\psi(x) = x + O(x^{1/2}\ln^2 x)$ [14], where ψ is the Chebyshev function, we suspect that the optimal order of $|c_n|$ is very close to $O(\ln n/n^{1/2})$. Figure 2 shows an example plot of c_n versus n, that illustrates the oscillatory behaviour of these constants. In addition, Smith has now numerically confirmed our conjecture for the first approximately 10^5 values of c_n [28].

In Figure 3 we have plotted the differences $\delta_n = c_n^2 - c_{n-1}c_{n+1}$ versus n, that

appear to support a decrease in $|c_n|$ with increasing n. In addition, the behaviour may indicate a correlation in the sign or other properties of the c_n's. Figure 4 plots the magnitude of the discrete Fourier transform applied to this sequence. This plot indicates underlying structure.

Our conjecture suggests that it may be worthwhile to study in detail the properties of the particular polylogarithm

$$L_{1/2}(z) \equiv \sum_{n=1}^{\infty} \frac{z^n}{n^{1/2}}, \tag{38}$$

such that $L_{1/2}(-1) = (\sqrt{2}-1)\zeta(1/2)$.

Previously, we obtained an expression for the Li/Keiper constants explicitly in terms of the Stieltjes constants [7]. We recall this and related results [7]:

Theorem

$$\lambda_n = 1-\frac{n}{2}(\ln\pi+2\ln 2-\gamma)+S_1(n)-\sum_{j=2}^{n}(-1)^j\binom{n}{j}j\sum_{h=1}^{j}\frac{1}{h}\sum_{\substack{j_1\geq 0,\ldots,j_h\geq 0\\ j_1+\cdots+j_h=j-h}}\prod_{b=1}^{h}\frac{\gamma_{j_b}}{j_b!}, \qquad n\geq 2, \tag{39}$$

$$S_2(n) = n\gamma-\sum_{j=2}^{n}(-1)^j\binom{n}{j}j\sum_{h=1}^{j}\frac{1}{h}\sum_{\substack{j_1\geq 0,\ldots,j_h\geq 0\\ j_1+\cdots+j_h=j-h}}\prod_{b=1}^{h}\frac{\gamma_{j_b}}{j_b!}, \qquad n\geq 2, \tag{40}$$

and

Theorem

$$\eta_{k-1} = (-1)^k k\sum_{h=1}^{k}\frac{1}{h}\sum_{\substack{j_1\geq 0,\ldots,j_h\geq 0\\ j_1+\cdots+j_h=k-h}}\prod_{b=1}^{h}\frac{\gamma_{j_b}}{j_b!}, \qquad k\geq 2. \tag{41}$$

From Lemma 2 we obtain the exact relation

Theorem

$$c_n = \gamma - \frac{1}{n}\sum_{j=2}^{n}(-1)^j \binom{n}{j} j \sum_{h=1}^{j}\frac{1}{h} \sum_{\substack{j_1\geq 0,\ldots,j_h\geq 0\\ j_1+\cdots+j_h=j-h}} \prod_{b=1}^{h}\frac{\gamma_{j_b}}{j_b!}, \qquad n\geq 2. \tag{42}$$

On the right side of Eq. (42), the constrained sum over the indices j_ℓ means that we have a partition of $k-h$ over the nonnegative integers. All such partitions are considered, meaning that their order does not matter. The number of such partitions is $\binom{n-1}{h-1}$ in η_{n-1} or c_n.

From Eq. (4) we have

$$\frac{z}{1-z}\zeta\left(\frac{1}{1-z}\right) = 1 + \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\gamma_n\left(\frac{z}{1-z}\right)^{n+1}. \tag{43}$$

Then from the definition (1) and performing various expansions, we have

$$F(z) = -\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\left[\sum_{j=0}^{\infty}\frac{(-1)^j}{j!}\gamma_j z^{j+1}\left(\sum_{m=0}^{\infty}z^m\right)^{j+1}\right]^n. \tag{44}$$

Carrying out the expansion in powers of z in this equation must necessarily return us to Eq. (42) for the coefficients c_n.

From the Hadamard product formula for the zeta function (e.g., [29]),

$$\zeta(s) = \frac{\exp(\ln 2\pi - 1 - \gamma/2)s}{2(s-1)\Gamma(s/2+1)}\prod_\rho\left(1-\frac{s}{\rho}\right)e^{s/\rho}, \tag{45}$$

we obtain

$$F(z) = \frac{\ln 2\pi - 1 - \gamma/2}{1-z} - \ln 2 - \ln\Gamma\left[\frac{3-2z}{2(1-z)}\right] + \sum_\rho\left\{\ln\left[1-\frac{1}{\rho(1-z)}\right]+\frac{1}{\rho(1-z)}\right\}. \tag{46}$$

Since by Eq. (10), $\sum_\rho 1/\rho \equiv \sigma_1 = \lambda_1$, we have

$$F(z) = \frac{\ln \pi}{2(1-z)} - \ln 2 - \ln \Gamma\left[\frac{3-2z}{2(1-z)}\right] + \sum_\rho \ln\left[1 - \frac{1}{\rho(1-z)}\right]. \tag{47}$$

The value $F(0) = \sum_\rho \ln[(\rho-1)/\rho] = 0$ obtains because the sum over all the complex zeros of ζ contains the pairs of ρ with $1-\rho$.

From the functional equation in the form $\zeta(z) = \pi^{z-1}2^z\Gamma(1-z)\zeta(1-z)\sin(\pi z/2)$, we obtain

$$F\left(\frac{1}{z}\right) = F(z) - \ln z + \frac{\ln(-\pi)}{z-1} + \frac{z}{z-1}\ln 2 + \ln\Gamma\left(\frac{1}{1-z}\right) + \ln\sin\left[\frac{\pi}{2}\frac{z}{(z-1)}\right]. \tag{48}$$

This equation should be very useful in obtaining results on the boundedness of the c_n's.

Discussion of the logarithmic derivative of ζ

This function has proved to be central in analytic number theory. Here we recall some known results and relate them to Eqs. (17), (18), and others.

We have (e.g., [27, 29]) in terms of the prime counting function $\pi(x)$

$$\ln \zeta(s) = s\int_2^\infty \frac{\pi(x)}{x(x^s-1)}dx, \qquad \text{Re } s > 1. \tag{49}$$

Then

$$\frac{\zeta'(s)}{\zeta(s)} = \int_2^\infty \frac{\pi(x)}{x(x^s-1)}dx - s\int_2^\infty \frac{x^{s-1}\pi(x)\ln x}{(x^s-1)^2}dx, \qquad \text{Re } s > 1. \tag{50}$$

Since the function π has steps, these induce changes in the coefficients η_j, hence in $S_2(n)$ or the c_n constants. In the common region of validity Re $s > 1 \cap |s-1| < 3$,

we have from Eqs. (17) and (49)

$$[(s-1)+1]\int_2^\infty \frac{\pi(x)}{x(x^s-1)}dx = -\ln(s-1) - \sum_{p=1}^\infty \frac{\eta_{p-1}}{p}(s-1)^p. \tag{51}$$

That is, we could write for instance

$$-\ln(s-1) - \sum_{p=1}^\infty \frac{\eta_{p-1}}{p}(s-1)^p = [(s-1)+1]\int_2^\infty dx \frac{\pi(x)}{x}\left\{\frac{1}{x-1} - \frac{x\ln x}{(x-1)^2}(s-1)\right.$$
$$\left. + \left[-\frac{x}{2}\frac{\ln^2 x}{(x-1)^2} + \frac{x^2 \ln^2 x}{(x-1)^3}\right](s-1)^2 + O[(s-1)^3]\right\}, \tag{52}$$

where of course by the prime number theorem $\pi(x) \sim x/\ln x$ as $x \to \infty$. This equation in powers of $s-1$ gives in principle an integral representation for each of the coefficients η_j.

We mention an important occurrence of the logarithmic derivative in numerical analysis. The reciprocal of this function is key in the classical Newton iteration for root finding, bringing in connections with discrete dynamical systems. Then one seeks the attracting fixed points of the associated Newtonian mapping. Therefore, from this point of view it is not unexpected that the logarithmic derivative should play an important role in determining zeros.

Summary and Brief Discussion

By way of Lemma 2, or equivalently from the use of the theory of polygamma functions, we have shown that the constants c_n of Eqs. (2) and (3) omit the leading growth $(1/2)\ln n$ of λ_n/n. We have presented additional analytic arguments, a conjecture, and partial numerical results that point to the decrease of $|c_n|$ with n. We

have pointed out the limited possibility of directly applying the Bieberbach conjecture because the function F of Eq. (1) is not univalent within the unit disc.

The quantity $S_2(n)$ is formed as the binomial sum of the alternating η_j values of Eq. (17). The latter is a correlated sequence. For, we have previously exhibited [7] the explicit summatory relation imposed upon the η's by the functional equation of either the zeta or xi functions. This relation implies that a given η_j is connected to all the other values η_{j+1}, η_{j+2}, $\ldots$.

In Appendix B we call out an integral representation of the alternating zeta function that may permit a joining of probabilisitic interpretation of the zeta function with Krein spectral shift functions. In turn, this may provide a useful link between Hardy space theory and inverse scattering theory. Though fairly independent of the approach of this paper, we believe it may be worth pointing this out to other investigators.

The importance of an explicit formula for $S_2(n)$ or c_n should not be overlooked. For instance, in principle, only improved estimation of the Stieltjes constants prevents verification of the Riemann hypothesis by way of either the Li criterion [22] or by way of Criterion (c) of Ref. [3]. Concerning the magnitudes $|c_n|$, any subexponential bound would serve to verify the Riemann hypothesis.

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Figure Captions

FIG. 1. In this semilogarithmic plot, the upper curve corresponds to values of $6/\pi^2\sqrt{n}$ versus n, and the lower to values of $|c_n|$ versus n.

FIG. 2. Plot of c_n versus n.

FIG. 3. Plot of the differences $\delta_n = c_n^2 - c_{n-1}c_{n+1}$ versus n.

FIG. 4. Plot of the magnitude of the discrete Fourier transform of the c_n sequence.

Appendix A: Examples of c_n in terms of the Stieltjes constants

Here, γ is the Euler constant and γ_k are the Stieltjes constants appearing in Eq. (4). We have

$$c_1 = \gamma, \qquad c_2 = \gamma - \gamma^2/2 - \gamma_1, \tag{A.1}$$

$$c_3 = \gamma - \gamma^2 + \frac{1}{3}\gamma^3 - 2\gamma_1 + \gamma\gamma_1 + \frac{1}{2}\gamma_2, \tag{A.2}$$

$$c_4 = \gamma^3 - \frac{1}{4}\gamma^4 - \frac{1}{2}\gamma^2(3+2\gamma_1) + \gamma(1+3\gamma_1 - \frac{1}{2}\gamma_2) + \frac{1}{6}[-3\gamma_1(6+\gamma_1) + 9\gamma_2 - \gamma_3], \tag{A.3}$$

and

$$c_5 = -\gamma^4 + \frac{1}{5}\gamma^5 + \gamma^3(2+\gamma_1) + \frac{1}{2}\gamma^2(-4 - 8\gamma_1 + \gamma_2) + \gamma[1 + \gamma_1(6+\gamma_1) - 2\gamma_2 + \frac{1}{6}\gamma_3]$$
$$+\frac{1}{24}[72\gamma_2 + 12\gamma_1(-8 - 4\gamma_1 + \gamma_2) - 16\gamma_3 + \gamma_4]. \tag{A.4}$$

The first few d_k's are given by

$$d_0 = \frac{1}{2}\ln\pi, \tag{A.5}$$

$$d_1 = -\gamma/2 - \ln 2, \tag{A.6}$$

$$d_2 = -\gamma + \frac{1}{8}\pi^2 - 2\ln 2, \tag{A.7}$$

$$d_3 = -3\gamma + \frac{3}{4}\pi^2 - 6\ln 2 - \frac{7}{4}\zeta(3), \tag{A.8}$$

$$d_4 = -12\gamma + \frac{9}{2}\pi^2 + \frac{\pi^4}{16} - 24\ln 2 - 21\zeta(3), \tag{A.9}$$

and

$$d_5 = -60\gamma + 30\pi^2 + \frac{5}{4}\pi^4 - 120\ln 2 - 210\zeta(3) - \frac{93}{4}\zeta(5). \tag{A.10}$$

Appendix B: The alternating zeta function in inverse spectral theory

We first recall the alternating zeta function

$$\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} = (1 - 2^{1-s})\zeta(s), \qquad \text{Re } s > 0, \quad s \neq 1, \tag{B.1}$$

this being one of the many analytic continuations of the Dirichlet series for the Riemann zeta function. Without going into the details, it turns out that this function can be written as an integral representation with the Krein spectral shift function [21] associated with the harmonic oscillator Hamiltonian on the line, with a Dirichlet boundary condition at the origin. As a Corollary, one may write [21]

$$(1 - 2^{1-s})\zeta(s) = s \int_0^{\infty} e^{-sx} \phi(x) dx, \qquad \text{Re } s > 0, \tag{B.2}$$

where

$$\phi(x) = \sum_{n=1}^{\infty} \chi_{[\ln(2n-1), \ln 2n]}(x), \tag{B.3}$$

and χ is the characteristic function of an interval. More generally, if the Dirichlet boundary condition is enforced at any other point x, a family of functions $\zeta(x, s)$ is generated. The points of discontinuity of $\zeta(x, s)$ satisfy a differential equation in x called the Dubrovin equation. This differential equation gives a curve in the space of analytic functions with the alternating zeta function divided by s as the initial value [21].

Now it is possible to represent the function [12]

$$\eta(s) \equiv \frac{(s-1)}{s^2}\zeta(s) = \int_0^{\infty} e^{-xs} \phi_1(x) dx, \qquad \text{Re } s > 0, \tag{B.4}$$

with the real-valued function

$$\phi_1(x) = \sum_{1 \le n \le e^x} (1 + \ln n - x). \qquad (B.5)$$

Then it is possible to introduce a family of probability densities with $x \in [0, \infty)$ as $p_\sigma(x) = \phi_1(x) \exp(-\sigma x)/\eta(\sigma)$ for $\sigma > 0$ [12]. The cumulants of p_σ can be written either in terms of the Stieltjes constants or the Li/Keiper constants at $\sigma = 1$ [7, 12]. Comparing Eqs. (B.2) with (B.4) and (B.3) with (B.5), it appears that it should be possible to combine a probabilistic setting for the zeta function with an inverse spectral theory. This point of view offers a connection between quantum dynamics and stochastic processes.

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